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NEWS 11	SEP 01	INPADOC: New family current-awareness alert (SDI) available
NEWS 12	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
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NEWS 14	SEP 14	STN Patent Forum to be held October 13, 2004, in Iselin, NJ
NEWS 15	SEP 27	STANDARDS will no longer be available on STN
NEWS 16	SEP 27	SWETSCAN will no longer be available on STN

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
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STRUCTURE FILE UPDATES:   26 SEP 2004  HIGHEST RN 752189-88-1
DICTIONARY FILE UPDATES:  26 SEP 2004  HIGHEST RN 752189-88-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> s 90780-53-3/rn
L1            1 90780-53-3/RN

=> s 87042-40-8/rn
L2            1 87042-40-8/RN

=> s 90780-52-2/rn
L3            1 90780-52-2/RN

=> s 356041-27-5/rn
L4            1 356041-27-5/RN

=> s 90906-41-5/rn
L5            1 90906-41-5/RN

=> s 90780-51-1/rn
L6            1 90780-51-1/RN

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L7            6 L1 OR L2 OR L3 OR L4 OR L5 OR L6

=> s l7 full
L8            6 L1 OR L2 OR L3 OR L4 OR L5 OR L6

=> d l8 1-6 sub bib abs

L8   ANSWER 1 OF 6  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   356041-27-5  REGISTRY
CN   4,7,10,13,16,20-Docosahexaenoic acid, 19-hydroxy-, (4Z,7Z,10Z,13Z,16Z,20E)-
      (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C22 H32 O3
SR   CA
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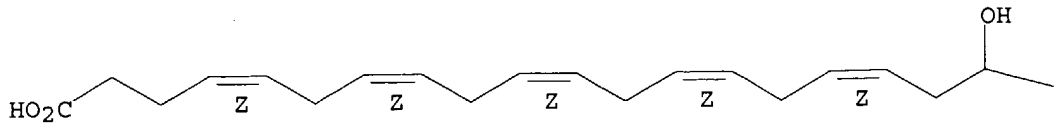
10663061

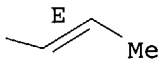
LC STN Files: CA, CAPLUS, USPAT2, USPATFULL
DT.CA CAplus document type: Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)

Double bond geometry as shown.

PAGE 1-A



PAGE 1-B



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:79114 CA
TI Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
IN Serhan, Charles N.; Colgan, Sean P.
PA The Brigham and Women's Hospital, USA
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053423	A2	20030703	WO 2002-US40586	20021218
	WO 2003053423	A3	20040226		

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	US 2003191184	A1	20031009	US 2002-323867	20021218
	US 2003195248	A1	20031016	US 2002-323591	20021218

PRAI US 2001-342138P 20011218

AB Methods to cause tissue, such as mucosal cells, to express increased amts. of bactericidal permeability increasing protein (BPI) are described. Various BPI inducing agents include eicosapentaenoic acid (EPA) analogs and docosahexaenoic acid (DHA) analogs. Thus, 18R-EPA analogs induced the

formation of BPI. Results demonstrated quant. PCR for BPI in epithelial cells.

REFERENCE 2

AN 135:190408 CA
TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		
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	US 2002055538	A1	20020509	US 2001-785866	20010216
	US 6670396	B2	20031230		
	EP 1296923	A2	20030402	EP 2001-910912	20010216
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	US 2004059144	A1	20040325	US 2003-663061	20030912
PRAI	US 2000-183078P	20000216			
	US 2000-238814P	20001006			
	US 2001-785866	20010216			
	WO 2001-US5196	20010216			

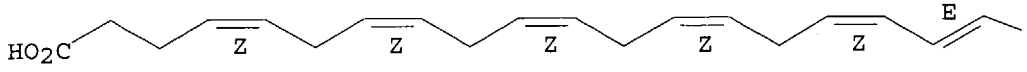
AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

L8 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2004 ACS on STN
RN **90906-41-5** REGISTRY
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (4Z,7Z,10Z,13Z,16Z,18E)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,7,10,13,16,18-Docosahexaenoic acid, 20-hydroxy-, (E,Z,Z,Z,Z,Z)-
FS STEREOSEARCH
DR 131391-58-7
MF C22 H32 O3
LC STN Files: CA, CAPLUS, CHEMCATS, CSCHEM, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); FORM (Formation, nonpreparative); PREP (Preparation)

Double bond geometry as shown.

PAGE 1-A



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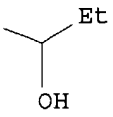

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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TI Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
IN Serhan, Charles N.; Colgan, Sean P.
PA The Brigham and Women's Hospital, USA
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053423	A2	20030703	WO 2002-US40586	20021218
	WO 2003053423	A3	20040226		
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PRAI US 2001-342138P 20011218

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TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		
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	US 2002055538	A1	20020509	US 2001-785866	20010216
	US 6670396	B2	20031230		
	EP 1296923	A2	20030402	EP 2001-910912	20010216
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003525880	T2	20030902	JP 2001-559832	20010216
	US 2004059144	A1	20040325	US 2003-663061	20030912
PRAI	US 2000-183078P	20000216			
	US 2000-238814P	20001006			
	US 2001-785866	20010216			
	WO 2001-US5196	20010216			

AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

REFERENCE 3

AN 120:265249 CA
TI High-performance liquid chromatography-thermospray mass spectrometry of epoxy polyunsaturated fatty acids and epoxyhydroxy polyunsaturated fatty acids from an incubation mixture of rat tissue homogenate
AU Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko
CS Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SO Journal of Chromatography, B: Biomedical Sciences and Applications (1994), 652(2), 123-36
CODEN: JCBBEP; ISSN: 1387-2273
DT Journal

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LA English
AB A method for the anal. of epoxy polyunsatd. fatty acids (EpPUFAs) and epoxyhydroxy polyunsatd. fatty acids (EpHPUFAs) in rat tissue homogenate, with homo-γ-linolenic acid (20:3,n-6), arachidonic acid (20:4,n-6), eicosapentaenoic acid (20:5,n-3) or docosahexaenoic acid (22:6,n-3) as a substrate, was developed. Extraction with dichloromethane at pH 4-5 and concentration in the presence of pyridine were performed. Spectral anal. of chromatograms obtained with HPLC-thermospray mass spectrometry showed the presence of EpPUFAs, EpHPUFAs and dihydroxy metabolites (DiHPUFAs) of EpPUFAs corresponding to each precursor fatty acid. On a selected-ion monitoring chromatogram, many EpPUFAs, EpHPUFAs and DiHPUFAs in an extract from an incubation mixture of each precursor fatty acid in aged rat tissue homogenate were detected simultaneously within 70 min. EpPUFAs and DiHPUFAs derived from 20:3 (n-6) or 20:5 (n-3) were detected in significant amts. From these results, a highly active cytochrome P 450 system or nonenzymic oxidative reactions in aged rat tissue homogenate were suggested.

REFERENCE 4

AN 119:265901 CA
TI Facile preparation and structural determination of monohydroxy derivatives of docosahexaenoic acid (HDoHE) by α-tocopherol-directed autoxidation
AU Reynaud, Denis; Thickitt, Christopher P.; Pace-Asciak, Cecil R.
CS Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.
SO Analytical Biochemistry (1993), 214(1), 165-70
CODEN: ANBCA2; ISSN: 0003-2697
DT Journal
LA English
AB Polyunsatd. fatty acids are oxidized through both enzymic and nonenzymic reactions into hydroxy derivs. With increasing interest in dietary manipulations through ingestion of the highly unsatd. fish oil fatty acids, eicosapentaenoic acid and docosahexaenoic acid (DHA), methods to measure their metabolism are required. In this study the authors report the simple and expedient α-tocopherol-directed autoxidative preparation of a series of monohydroxy derivs. of DHA to provide a relatively homogeneous hydroxylation along each of the double bonds of the fatty substrate. Products were purified by high-performance liquid chromatog. (HPLC) and their structures elucidated by the characteristic fragmentation pattern of the hydrogenated Me ester trimethylsilyl ether derivs. by gas chromatog.-mass spectrometry. Nine products were isolated in 20.2% yield overall, ranging from 1.55 to 4.14% yield of isolated compound These were identified as 7, 8, 10, 11, 13, 14, 16, 17, and 20-HDoHEs (monohydroxydocosahexaenoic acids). Two of these products (14- and 17-HDoHE) could not be separated under the HPLC conditions used but were clearly distinguished using selected ion chromatog. by their distinct mass spectral fragmentation. This method is highly suitable for the generation of stds. to investigate the metabolism of DHA in tissues.

REFERENCE 5

AN 114:39806 CA
TI Stereochemical analysis of hydroxylated docosahexaenoates produced by human platelets and rat brain homogenate
AU Kim, H. Y.; Karanian, J. W.; Shingu, T.; Salem, N., Jr.
CS Sect. Anal. Chem., NIAAA, Bethesda, MD, 20892, USA
SO Prostaglandins (1990), 40(5), 473-90
CODEN: PRGLBA; ISSN: 0090-6980
DT Journal
LA English

10663061

AB The stereochem. configuration of hydroxylated products of docosahexaenoic acid (22:6ω3) formed by human platelets and rat brain homogenate were characterized for the first time. Chiral phase HPLC was employed along with autoxidized 22:6ω3 as reference material. The 14- and 11-hydroy 22:6ω3 (HDHE) products produced by human platelets were in the S configuration. Rat brain homogenate produced all of the 10 possible positional isomers when incubated with 22:6ω3. Their retention behavior on the reversed and chiral phase HPLC columns and GC/MS/EI anal. indicated that they were 20-, 17-, 16-, 14-, 13-, 11-, 10-, 8-, 7- and 4-HDHE. However, stereochem. anal. revealed that each positional isomer was a racemic mixture, suggesting that these were not formed by lipoxygenation but mainly by peroxidn. process.

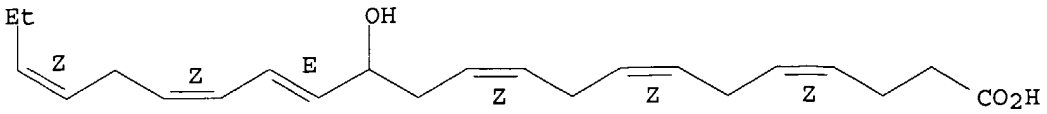
REFERENCE 6

AN 101:35331 CA
TI Autooxidation of docosahexaenoic acid: analysis of ten isomers of hydroxydocosahexaenoate
AU VanRollins, Mike; Murphy, Robert C.
CS Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SO Journal of Lipid Research (1984), 25(5), 507-17
CODEN: JLPRAW; ISSN: 0022-2275
DT Journal
LA English
AB Docosahexaenoic acid, an n-3 essential fatty acid, is enzymically converted by platelets, basophils, and liver microsomes into metabolites containing conjugated diens with allylic hydroxyl groups. To help identify these metabolites, stds. were prepared by autoxidn. of docosahexaenoic acid. After isolation by reverse phase and normal phase high-performance chromatog. (HPLC), 10 hydroxy isomers of docosahexaenoic acid were identified by capillary gas-liquid chromatog., UV spectroscopy, and mass spectrometry. From these studies and reported elution orders for similar metabolites derived from linoleic, linolenic, and arachidonic acids, 2 basic HPLC elution patterns became apparent. Under reverse phase chromatog. conditions, the distance of the trans-double bond from the carboxyl group was the critical parameter in determining the elution order. Under silicic acid chromatog. conditions, the distance of the hydroxyl from the carbomethoxy group seemed to determine the elution order. The dramatic difference in selectivity between reverse and normal phase HPLC of the hydroxy acids provides critical information useful for identifying endogenous metabolites.

L8 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2004 ACS on STN
RN **90780-53-3** REGISTRY
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (4Z,7Z,10Z,14E,16Z,19Z)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,7,10,14,16,19-Docosahexaenoic acid, 13-hydroxy-, (E,Z,Z,Z,Z,Z)-
FS STEREOSEARCH
DR 131391-60-1
MF C22 H32 O3
LC STN Files: CA, CAPLUS, CHEMCATS, CSCHEM, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PRP (Properties)

Double bond geometry as shown.

10663061



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:177077 CA
TI Novel Docosatrienes and 17S-Resolvins Generated from Docosahexaenoic Acid in Murine Brain, Human Blood, and Glial Cells
AU Hong, Song; Gronert, Karsten; Devchand, Pallavi R.; Moussignac, Rose-Laure; Serhan, Charles N.
CS Perioperative and Pain Medicine, Department of Anesthesiology, Center for Experimental Therapeutics and Reperfusion Injury, Brigham and Women's Hospital and Harvard Medical School, Boston, MA, 02115, USA
SO Journal of Biological Chemistry (2003), 278(17), 14677-14687
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
AB Docosahexaenoic acid (DHA, C22:6) is highly enriched in brain, synapses, and retina and is a major ω-3 fatty acid. Deficiencies in this essential fatty acid are reportedly associated with neuronal function, cancer, and inflammation. Here, using new lipid analyses employing high performance liquid chromatog. coupled with a photodiode-array detector and a tandem mass spectrometer, a novel series of endogenous mediators was identified in blood, leukocytes, brain, and glial cells as 17S-hydroxy-containing docosanoids denoted as docosatrienes (the main bioactive member of the series was 10,17S-docosatriene) and 17S series resolvins. These novel mediators were biosynthesized via epoxide-containing intermediates and proved potent (pico- to nanomolar range) regulators of both leukocytes reducing infiltration in vivo and glial cells blocking their cytokine production These results indicate that DHA is the precursor to potent protective mediators generated via enzymic oxygenations to novel docosatrienes and 17S series resolvins that each regulate events of interest in inflammation and resolution
RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 2

AN 139:79114 CA
TI Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
IN Serhan, Charles N.; Colgan, Sean P.
PA The Brigham and Women's Hospital, USA
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053423	A2	20030703	WO 2002-US40586	20021218
	WO 2003053423	A3	20040226		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

US	2003191184	A1	20031009	US 2002-323867	20021218
US	2003195248	A1	20031016	US 2002-323591	20021218

PRAI US 2001-342138P 20011218

AB Methods to cause tissue, such as mucosal cells, to express increased amts. of bactericidal permeability increasing protein (BPI) are described. Various BPI inducing agents include eicosapentaenoic acid (EPA) analogs and docosahexaenoic acid (DHA) analogs. Thus, 18R-EPA analogs induced the formation of BPI. Results demonstrated quant. PCR for BPI in epithelial cells.

REFERENCE 3

AN 135:190408 CA
TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US	2002055538	A1	20020509	US 2001-785866	20010216
US	6670396	B2	20031230		
EP	1296923	A2	20030402	EP 2001-910912	20010216

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP	2003525880	T2	20030902	JP 2001-559832	20010216
US	2004059144	A1	20040325	US 2003-663061	20030912

PRAI US 2000-183078P 20000216
US 2000-238814P 20001006
US 2001-785866 20010216
WO 2001-US5196 20010216

AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and

10663061

15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

REFERENCE 4

AN 121:78737 CA
TI Polyunsaturated-fatty-acid oxidation in Hydra: regioselectivity, substrate-dependent enantioselectivity and possible biological role
AU Di Marzo, Vincenzo; Gianfrani, Carmen; De Petrocellis, Luciano; Milone, Alfredo; Cimino, Guido
CS Ist. Chim. Mol. Interesse Biol., CNR, Arco Felice, 80072, Italy
SO Biochemical Journal (1994), 300(2), 501-7
CODEN: BIJOAK; ISSN: 0264-6021
DT Journal
LA English
AB A novel and abundant lipoxygenase-like activity converting cis-eicosa-5,8,11,14-tetraenoic acid (arachidonic acid) into (11R)-hydroxyeicosatetraenoic acid has been recently described in homogenates of the freshwater hydrozoan Hydra vulgaris. In this study, other substrates for this enzyme were selected from the polyunsatd. fatty acids (PUFAs) present in H. vulgaris, and the chemical natures of the hydroperoxy and hydroxy derivs. produced, as well as the activity of some of the latter on hydroid tentacle regeneration, were investigated. The highest conversion among C20 fatty acids was observed for arachidonic acid, and among C18 fatty acids for cis-octadeca-9,12,15- and cis-octadeca-6,9,12-trienoic (α- and γ-linolenic) acids. Cis double bonds on the 10th C atom from the aliphatic end of the substrate (e.g. C-9, C-11, and C-13 resp. in C18, C20, and C22 PUFAs) were regiospecifically peroxidized. Conversely, trans-octadeca-9,12-dienoic (linelaidic) acid was not a substrate for lipoxygenase activity. Enantioselectivity of lipoxygenation depended on the degree of unsatn. of the substrate, with the amount of the R enantiomer increasing when passing, for example, from cis-eicosa-11,14-dienoic to cis-eicosa-5,8,11,14,17-pentaenoic acid. Regiospecific formation of keto acids was observed only when incubating C18 PUFAs. Com. available hydroxyacids corresponding to the reaction products of some of the most abundant H. vulgaris PUFAs were tested for effects on Hydra tentacle regeneration. An enhancement of average tentacle number, in a fashion depending on the stereochem. and on the number of double bonds, was found for 2 compds., thus suggesting for the 11-lipoxygenase-like enzyme a role in the production of metabolites potentially active in the control of hydroid regenerative processes.

REFERENCE 5

AN 119:265901 CA
TI Facile preparation and structural determination of monohydroxy derivatives of docosahexaenoic acid (HDoHE) by α-tocopherol-directed autoxidation
AU Reynaud, Denis; Thickitt, Christopher P.; Pace-Asciak, Cecil R.
CS Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.
SO Analytical Biochemistry (1993), 214(1), 165-70
CODEN: ANBCA2; ISSN: 0003-2697
DT Journal
LA English
AB Polyunsatd. fatty acids are oxidized through both enzymic and nonenzymic reactions into hydroxy derivs. With increasing interest in dietary manipulations through ingestion of the highly unsatd. fish oil fatty acids, eicosapentaenoic acid and docosahexaenoic acid (DHA), methods to measure their metabolism are required. In this study the authors report the

simple and expedient α-tocopherol-directed autoxidative preparation of a series of monohydroxy derivs. of DHA to provide a relatively homogeneous hydroxylation along each of the double bonds of the fatty substrate. Products were purified by high-performance liquid chromatog. (HPLC) and their structures elucidated by the characteristic fragmentation pattern of the hydrogenated Me ester trimethylsilyl ether derivs. by gas chromatog.-mass spectrometry. Nine products were isolated in 20.2% yield overall, ranging from 1.55 to 4.14% yield of isolated compound These were identified as 7, 8, 10, 11, 13, 14, 16, 17, and 20-HDoHEs (monohydroxydocosahexaenoic acids). Two of these products (14- and 17-HDoHE) could not be separated under the HPLC conditions used but were clearly distinguished using selected ion chromatog. by their distinct mass spectral fragmentation. This method is highly suitable for the generation of stds. to investigate the metabolism of DHA in tissues.

REFERENCE 6

AN 114:39806 CA
TI Stereochemical analysis of hydroxylated docosahexaenoates produced by human platelets and rat brain homogenate
AU Kim, H. Y.; Karanian, J. W.; Shingu, T.; Salem, N., Jr.
CS Sect. Anal. Chem., NIAAA, Bethesda, MD, 20892, USA
SO Prostaglandins (1990), 40(5), 473-90
CODEN: PRGLBA; ISSN: 0090-6980
DT Journal
LA English
AB The stereochem. configuration of hydroxylated products of docosahexaenoic acid (22:6ω3) formed by human platelets and rat brain homogenate were characterized for the first time. Chiral phase HPLC was employed along with autoxidized 22:6ω3 as reference material. The 14- and 11-hydroy 22:6ω3 (HDHE) products produced by human platelets were in the S configuration. Rat brain homogenate produced all of the 10 possible positional isomers when incubated with 22:6ω3. Their retention behavior on the reversed and chiral phase HPLC columns and GC/MS/EI anal. indicated that they were 20-, 17-, 16-, 14-, 13-, 11-, 10-, 8-, 7- and 4-HDHE. However, stereochem. anal. revealed that each positional isomer was a racemic mixture, suggesting that these were not formed by lipoxygenation but mainly by peroxidn. process.

REFERENCE 7

AN 101:35331 CA
TI Autooxidation of docosahexaenoic acid: analysis of ten isomers of hydroxydocosahexaenoate
AU VanRollins, Mike; Murphy, Robert C.
CS Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SO Journal of Lipid Research (1984), 25(5), 507-17
CODEN: JLPRAW; ISSN: 0022-2275
DT Journal
LA English
AB Docosahexaenoic acid, an n-3 essential fatty acid, is enzymically converted by platelets, basophils, and liver microsomes into metabolites containing conjugated diens with allylic hydroxyl groups. To help identify these metabolites, stds. were prepared by autoxidn. of docosahexaenoic acid. After isolation by reverse phase and normal phase high-performance chromatog. (HPLC), 10 hydroxy isomers of docosahexaenoic acid were identified by capillary gas-liquid chromatog., UV spectroscopy, and mass spectrometry. From these studies and reported elution orders for similar metabolites derived from linoleic, linolenic, and arachidonic acids, 2 basic HPLC elution patterns became apparent. Under reverse phase chromatog. conditions, the distance of the trans-double bond from the carboxyl group was the critical parameter in determining the elution order. Under

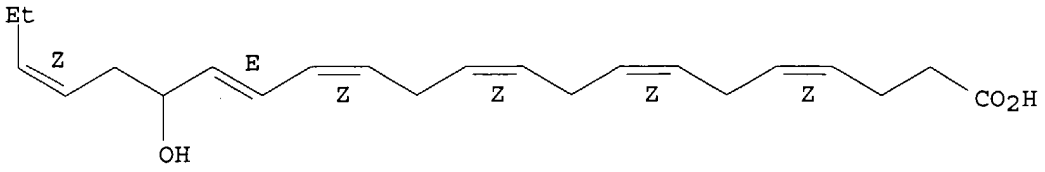
silicic acid chromatog. conditions, the distance of the hydroxyl from the carbomethoxy group seemed to determine the elution order. The dramatic difference in selectivity between reverse and normal phase HPLC of the hydroxy acids provides critical information useful for identifying endogenous metabolites.

REFERENCE 8

AN 101:19194 CA
TI Oxidation of docosahexaenoic acid by rat liver microsomes
AU VanRollins, Mike; Baker, Rodney C.; Sprecher, Howard W.; Murphy, Robert C.
CS Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SO Journal of Biological Chemistry (1984), 259(9), 5776-83
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA English
AB [1-14C]docosahexaenoic acid (n-3) was incubated at 37° for 30 min in the presence of rat liver microsomes and 1 mM NADPH. The products were isolated by using organic solvent extns., and reverse phase and normal phase HPLC. Isolates were identified by UV spectroscopy, capillary gas-liquid chromatog., and gas chromatog.-mass spectrometer. The major metabolites were: 19,20-, 16,17-, 13,14-, 10,11-, and 7,8-dihydroxydocosapentaenoic acids, 22-hydroxydocosahexaenoic acid, and 21-hydroxydocosahexaenoic acid. The minor metabolites were 17-hydroxy-4,7,10,13,15,19-, 16-hydroxy-4,7,10,17,19-, 14-hydroxy-4,7,10,12,-16,19-, 13-hydroxy-4,7,10,14,16,19-, 11-hydroxy-4,7,9,13,16,19-, 10-hydroxy-4,7,11,13,16,19-,8-hydroxy-4,6,10,13,16,19-, and 7-hydroxy-4,8,10,13,16,19-docosahexaenoic acids. These metabolites of docosahexaenoic acid resulted from 4 distinct classes of oxidation, ω-hydroxylations, (ω-1)-hydroxylations, epoxidns., and lipoxygenase-like hydroxylations. The similarity of these product profiles to those reported for comparable microsomal incubations with other essential fatty acids suggest that microsome cytochrome P 450 monooxygenases were involved.

L8 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2004 ACS on STN
RN **90780-52-2** REGISTRY
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (4Z,7Z,10Z,13Z,15E,19Z)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,7,10,13,15,19-Docosahexaenoic acid, 17-hydroxy-, (E,Z,Z,Z,Z,Z)-
FS STEREOSEARCH
DR 131485-67-1
MF C22 H32 O3
LC STN Files: CA, CANCERLIT, CAPLUS, CHEMCATS, CSCHEM, MEDLINE, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process)

Double bond geometry as shown.



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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

17 REFERENCES IN FILE CA (1907 TO DATE)
17 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:79114 CA
TI Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
IN Serhan, Charles N.; Colgan, Sean P.
PA The Brigham and Women's Hospital, USA
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053423	A2	20030703	WO 2002-US40586	20021218
	WO 2003053423	A3	20040226		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003191184	A1	20031009	US 2002-323867	20021218
	US 2003195248	A1	20031016	US 2002-323591	20021218
PRAI	US 2001-342138P		20011218		

AB Methods to cause tissue, such as mucosal cells, to express increased amts. of bactericidal permeability increasing protein (BPI) are described. Various BPI inducing agents include eicosapentaenoic acid (EPA) analogs and docosahexaenoic acid (DHA) analogs. Thus, 18R-EPA analogs induced the formation of BPI. Results demonstrated quant. PCR for BPI in epithelial cells.

REFERENCE 2

AN 136:147175 CA
TI Monohydroxylated fatty acid content in peripheral blood mononuclear cells and immune status of people at long times after the Chernobyl accident
AU Chumak, Anatoliy; Thevenon, Chantal; Gulaya, Nadya; Guichardant, Michel; Margitich, Victor; Bazyka, Dimitry; Kovalenko, Alexander; Lagarde, Michel; Prigent, Annie-France
CS INSERM, Biochimie et Pharmacologie INSA Lyon, Villeurbanne, 69621, Fr.
SO Radiation Research (2001), 156(5, Pt. 1), 476-487
CODEN: RAREAE; ISSN: 0033-7587
PB Radiation Research Society
DT Journal
LA English
AB The monohydroxylated fatty acid content of peripheral blood mononuclear cells from 23 cleanup workers and 16 unexposed individuals was studied in relation to their immune status after the Chernobyl accident. Men with absorbed doses below 0.32 Gy showed higher levels of free and esterified 12-hydroxyeicosatetraenoic acid (12-HETE) than unexposed men, whereas 15-HETE and the 17-hydroxy derivative of C22 fatty acid (17-OH 22), either

free or esterified in phospholipids, were increased in a dose-dependent manner. The percentage of CD4-pos. cells was also increased significantly in heavily irradiated men, whereas the percentage of CD8-pos. cells tended to decrease with dose. Furthermore, the absolute count of CD4-pos. cells was correlated pos. with the amount of esterified 15-HETE in the phospholipid fraction of the mononuclear cells and with the total 15-HETE. These results show for the first time that the accumulation of autoxidized/lipoxygenase products of polyunsatd. fatty acids in the mononuclear cells of irradiated individuals was associated with immune imbalance. This may be the basis for certain late effects of radiation such as autoimmune disorders, somatic and neoplastic diseases, and early aging.

RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 3

AN 135:190408 CA
TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	US 2002055538	A1	20020509	US 2001-785866	20010216
	US 6670396	B2	20031230		
	EP 1296923	A2	20030402	EP 2001-910912	20010216
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003525880	T2	20030902	JP 2001-559832	20010216
	US 2004059144	A1	20040325	US 2003-663061	20030912

PRAI US 2000-183078P 20000216
US 2000-238814P 20001006
US 2001-785866 20010216
WO 2001-US5196 20010216

AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

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REFERENCE 4

AN 129:202364 CA
TI N-3 fatty acid deficiency in the rat pineal gland: effects on phospholipid molecular species composition and endogenous levels of melatonin and lipoxygenase products
AU Zhang, Hongjian; Hamilton, Jillonne H.; Salem, Norman, Jr.; Kim, Hee-Yong
CS Section of Mass Spectrometry, National Institute on Alcohol Abuse and Alcoholism, National Institutes of Health, Rockville, MD, 20852, USA
SO Journal of Lipid Research (1998), 39(7), 1397-1403
CODEN: JLPRAW; ISSN: 0022-2275
PB Lipid Research, Inc.
DT Journal
LA English
AB N-3 essential fatty acid deficiency affects a number of biol. and physiol. processes. In this study, the authors investigated the effect of n-3 essential fatty acid status on two key pineal biochem. functions, melatonin production and lipoxygenation, using pineal glands from rats given an n-3-adequate or n-3-deficient diet. The pineal total lipid profile and phospholipid mol. species distribution altered by n-3 deficiency were evaluated in parallel. In pineal glands from n-3-deficient rats, an 87% reduction of 22:6n-3 (docosahexaenoic acid) was observed, and this decrease was accompanied by increases in 22:4n-6 (docosatetraenoic acid, 3-fold), 22:5n-6 (docosapentaenoic acid, 12-fold), and 20:4n-6 (arachidonic acid, 48%). The significant decrease of 22:6n-3 containing species in phosphatidylcholine (PC), phosphatidylethanolamine (PE), and phosphatidylserine (PS) was also evident. These decreases in 22:6n-3 containing PL species were compensated by substantial accumulations of 22:4n-6 or 22:5n-6 and slight increases in 20:4n-6 containing PL species in PC and PE. In PS, however, the accumulation of n-6 species was not adequate to compensate for the loss of 22:6n-3 species. N-3 deficiency significantly reduced non-esterified 20:4n-6 and 22:6n-3 levels in pineals (25% and 65%, resp.). Concomitantly, the endogenous 12-HETE level decreased by 35% in deficient pineals. In contrast, n-3 deficiency led to a more than 60% increase in the daytime pineal melatonin level. In conclusion, n-3 fatty acid deficiency not only has profound effects on pineal lipid profiles but also on pineal biochem. activities. These results suggest that n-3 fatty acids may play a critical role in regulating pineal function.
RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 5

AN 124:26230 CA
TI Biosynthesis of docosanoids by human platelet: Cardiovascular properties
AU Karanian, John W.; Kim, Hee Yong; Salem, Norman Jr.
CS Laboratory Membrane Biochemistry and Biophysics, DICBR/NIAAA, Rockville, MD, 20852, USA
SO Cardiovascular Disease 2: Cellular and Molecular Mechanisms, Prevention, and Treatment, [Proceedings of the Washington International Spring Symposium], 14th, Washington, D. C., June 6-10, 1994 (1995), Meeting Date 1994, 269-77. Editor(s): Gallo, Linda L. Publisher: Plenum, New York, N. Y.
CODEN: 61ZNA9
DT Conference
LA English
AB A reliable purification and quantification method is presented that was used to characterize the metabolism and production of the hydroxylated derivs. of 22:5n3, 22:6n3, 22:5n5 and 22:5n6 from mammalian platelets. Their biol. properties in platelet and vascular smooth muscle cell function is

discussed.

REFERENCE 6

AN 121:277471 CA
TI Inhibitory effects of n-6 and n-3 hydroxy fatty acids on thromboxane (U46619)-induced smooth muscle contraction
AU Karanian, J. W.; Kim, H. Y.; Salem, Norman, Jr.
CS Lab. Membrane Biochem. and Biophysics, Natl. Inst. Alcohol Abuse and Alcoholism, Bethesda, MD, USA
SO Journal of Pharmacology and Experimental Therapeutics (1994), 270(3), 1105-9
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA English
AB Mammalian platelets are capable of enzymically producing a number of n-6 and n-3 hydroxy fatty acids. Human platelet suspensions produce two major docosahexaenoic acid (22:6n3) metabolites, namely, 11-OH- and 14-OH-22:6n3. The hydroxy fatty acids which were formed by human platelets and purified by high performance liquid chromatog. specifically antagonize the contractile effects of a thromboxane mimetic, U46619, in airway, visceral and, especially, in the vascular smooth muscle prepns. studied.
The efficacy of OH-22:6n3 (IC25 = 1.1 μM) was compared to other n-6 and n-3 hydroxy fatty acids in the rat aortic ring preparation The OH-22:6n3 was significantly more potent with the exception of OH-22:5n3. The rank order of their potency was 14-OH-22:5n3 ≥ 14-OH-22:6n3 > 17-OH-22:6n3 ≥ 11-OH-22:6n3 ≥ 11-OH-22:5n3 > 12-OH-20:5n3 ≥ 12-OH-20:4n6 ≥ 14-OH-22:5n6 > 13-OH-18:2n6 > 14-OH-22:5n5. Antagonism of thromboxane effects may be an important aspect of the biol. function of 22-carbon n-3 hydroxylated fatty acids in the platelet-vascular smooth muscle cell interactions.

REFERENCE 7

AN 120:265249 CA
TI High-performance liquid chromatography-thermospray mass spectrometry of epoxy polyunsaturated fatty acids and epoxyhydroxy polyunsaturated fatty acids from an incubation mixture of rat tissue homogenate
AU Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko
CS Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SO Journal of Chromatography, B: Biomedical Sciences and Applications (1994), 652(2), 123-36
CODEN: JCBBEP; ISSN: 1387-2273
DT Journal
LA English
AB A method for the anal. of epoxy polyunsatd. fatty acids (EpPUFAs) and epoxyhydroxy polyunsatd. fatty acids (EpHPUFAs) in rat tissue homogenate, with homo-γ-linolenic acid (20:3,n-6), arachidonic acid (20:4,n-6), eicosapentaenoic acid (20:5,n-3) or docosahexaenoic acid (22:6,n-3) as a substrate, was developed. Extraction with dichloromethane at pH 4-5 and concentration in the presence of pyridine were performed. Spectral anal. of chromatograms obtained with HPLC-thermospray mass spectrometry showed the presence of EpPUFAs, EpHPUFAs and dihydroxy metabolites (DiHPUFAs) of EpPUFAs corresponding to each precursor fatty acid. On a selected-ion monitoring chromatogram, many EpPUFAs, EpHPUFAs and DiHPUFAs in an extract from an incubation mixture of each precursor fatty acid in aged rat tissue homogenate were detected simultaneously within 70 min. EpPUFAs and DiHPUFAs derived from 20:3 (n-6) or 20:5 (n-3) were detected in significant amts. From these results, a highly active cytochrome P 450 system or nonenzymic oxidative reactions in aged rat tissue homogenate

were suggested.

REFERENCE 8

AN 119:265901 CA
TI Facile preparation and structural determination of monohydroxy derivatives of docosahexaenoic acid (HDoHE) by α-tocopherol-directed autoxidation
AU Reynaud, Denis; Thickitt, Christopher P.; Pace-Asciak, Cecil R.
CS Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.
SO Analytical Biochemistry (1993), 214(1), 165-70
CODEN: ANBCA2; ISSN: 0003-2697
DT Journal
LA English
AB Polyunsatd. fatty acids are oxidized through both enzymic and nonenzymic reactions into hydroxy derivs. With increasing interest in dietary manipulations through ingestion of the highly unsatd. fish oil fatty acids, eicosapentaenoic acid and docosahexaenoic acid (DHA), methods to measure their metabolism are required. In this study the authors report the simple and expedient α-tocopherol-directed autoxidative preparation of a series of monohydroxy derivs. of DHA to provide a relatively homogeneous hydroxylation along each of the double bonds of the fatty substrate. Products were purified by high-performance liquid chromatog. (HPLC) and their structures elucidated by the characteristic fragmentation pattern of the hydrogenated Me ester trimethylsilyl ether derivs. by gas chromatog.-mass spectrometry. Nine products were isolated in 20.2% yield overall, ranging from 1.55 to 4.14% yield of isolated compound These were identified as 7, 8, 10, 11, 13, 14, 16, 17, and 20-HDoHEs (monohydroxydocosahexaenoic acids). Two of these products (14- and 17-HDoHE) could not be separated under the HPLC conditions used but were clearly distinguished using selected ion chromatog. by their distinct mass spectral fragmentation. This method is highly suitable for the generation of stds. to investigate the metabolism of DHA in tissues.

REFERENCE 9

AN 117:187518 CA
TI High-performance liquid chromatography-thermospray mass spectrometry of hydroperoxy polyunsaturated fatty acid acetyl derivatives
AU Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko; Ishikawa, Fumio
CS Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SO Journal of Chromatography (1992), 579(1), 25-36
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB A method for the anal. of hydroperoxy polyunsatd. fatty acids was developed. The hydroperoxy groups were acetylated by acetic anhydride, and the mixture was partially purified on a Sep-Pak C18 cartridge and analyzed by high-performance liquid chromatog. with thermospray mass spectrometry. Generally, the base ion, [M + H - n(60)]+ or [M + H - n(60) - n(H2O)]+, is produced through elimination of acetic acid or water (n = number of hydroperoxy groups). The detection limit for these derivs. was approx. 1 pmol at concns. of hydroperoxy polyenoic acids prior to derivatization. Using this method, many hydroxy and hydroperoxy polyunsatd. fatty acid derivs. could be detected simultaneously within 30 min on a selected-ion monitoring detection chromatogram without a gradient system. The assay was successfully applied to hydroxy and hydroperoxy polyunsatd. fatty acids from an incubation mixture of rat brain homogenate to which polyunsatd. fatty acids has been added.

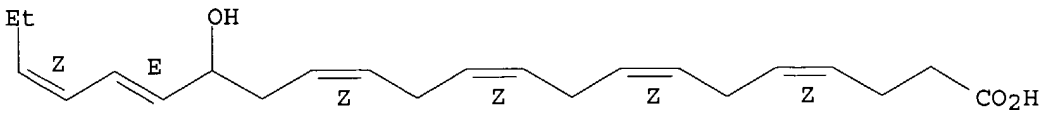
REFERENCE 10

10663061

AN 116:211313 CA
TI Identification and egg hatching activity of monohydroxy fatty acid eicosanoids in the barnacle Balanus balanoides
AU Hill, E. M.; Holland, D. L.
CS Sch. Ocean Sci., Univ. Coll. North Wales, Anglesey, LL59 5EY, UK
SO Proceedings of the Royal Society of London, Series B: Biological Sciences (1992), 247(1318), 41-6
CODEN: PRLBA4; ISSN: 0080-4649
DT Journal
LA English
AB Monohydroxy fatty acids (MHFAs) were isolated from homogenates of the barnacle B. balanoides and identified by gas chromatog.-mass spectrometry (GC-MS) as 14- and 17-hydroxy docosahexaenoic acids, 8-, 11-, 12-, 15- and 18-hydroxy eicosapentaenoic acids, 13- and 16-hydroxyoctadecatrienoic acids, and 9-, 13- and 15-hydroxyoctadecadienoic acids. Each monohydroxy fatty acid was tested for egg hatching activity in a bioassay using Elminius modestus egg masses, but 8-hydroxy-5, 9, 11, 14, 17-eicosapentaenoic acid (8-HEPE) was the only MHFA with barnacle egg hatching activity. Studies on the egg hatching activity of MHFAs prepared from the oxidation of polyunsatd. fatty acids showed that activity was confined to the 8-hdyroxy isomer of eicosapentaenoic acid and arachidonic acid, and that unsatn. at C5 and C14, but not C17, was essential for activity. In addition, the 8(R) conformation is necessary for activity, as 8(R)-HEPE caused egg hatching at 10-7M, whereas the enantiomer 8(S)-HEPE was inactive.

L8 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2004 ACS on STN
RN **90780-51-1** REGISTRY
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (4Z,7Z,10Z,13Z,17E,19Z)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,7,10,13,17,19-Docosahexaenoic acid, 16-hydroxy-, (E,Z,Z,Z,Z,Z)-
FS STEREOSEARCH
DR 131391-59-8
MF C22 H32 O3
LC STN Files: CA, CAPLUS, CHEMCATS, CSCHEM, USPAT2, USPATFULL
DT.CA CAplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)

Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:79114 CA
TI Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
IN Serhan, Charles N.; Colgan, Sean P.

10663061

PA The Brigham and Women's Hospital, USA
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053423	A2	20030703	WO 2002-US40586	20021218
	WO 2003053423	A3	20040226		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

	US 2003191184	A1	20031009	US 2002-323867	20021218
	US 2003195248	A1	20031016	US 2002-323591	20021218

PRAI US 2001-342138P 20011218

AB Methods to cause tissue, such as mucosal cells, to express increased amts. of bactericidal permeability increasing protein (BPI) are described. Various BPI inducing agents include eicosapentaenoic acid (EPA) analogs and docosahexaenoic acid (DHA) analogs. Thus, 18R-EPA analogs induced the formation of BPI. Results demonstrated quant. PCR for BPI in epithelial cells.

REFERENCE 2

AN 135:190408 CA
TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

	US 2002055538	A1	20020509	US 2001-785866	20010216
	US 6670396	B2	20031230		
	EP 1296923	A2	20030402	EP 2001-910912	20010216

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

	JP 2003525880	T2	20030902	JP 2001-559832	20010216
	US 2004059144	A1	20040325	US 2003-663061	20030912

10663061

PRAI US 2000-183078P 20000216
US 2000-238814P 20001006
US 2001-785866 20010216
WO 2001-US5196 20010216

AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

REFERENCE 3

AN 119:265901 CA
TI Facile preparation and structural determination of monohydroxy derivatives of docosahexaenoic acid (HDoHE) by α-tocopherol-directed autoxidation
AU Reynaud, Denis; Thickitt, Christopher P.; Pace-Asciak, Cecil R.
CS Res. Inst., Hosp. Sick Child., Toronto, ON, M5G 1X8, Can.
SO Analytical Biochemistry (1993), 214(1), 165-70
CODEN: ANBCA2; ISSN: 0003-2697
DT Journal
LA English
AB Polyunsatd. fatty acids are oxidized through both enzymic and nonenzymic reactions into hydroxy derivs. With increasing interest in dietary manipulations through ingestion of the highly unsatd. fish oil fatty acids, eicosapentaenoic acid and docosahexaenoic acid (DHA), methods to measure their metabolism are required. In this study the authors report the simple and expedient α-tocopherol-directed autoxidative preparation of a series of monohydroxy derivs. of DHA to provide a relatively homogeneous hydroxylation along each of the double bonds of the fatty substrate. Products were purified by high-performance liquid chromatog. (HPLC) and their structures elucidated by the characteristic fragmentation pattern of the hydrogenated Me ester trimethylsilyl ether derivs. by gas chromatog.-mass spectrometry. Nine products were isolated in 20.2% yield overall, ranging from 1.55 to 4.14% yield of isolated compound These were identified as 7, 8, 10, 11, 13, 14, 16, 17, and 20-HDoHEs (monohydroxydocosahexaenoic acids). Two of these products (14- and 17-HDoHE) could not be separated under the HPLC conditions used but were clearly distinguished using selected ion chromatog. by their distinct mass spectral fragmentation. This method is highly suitable for the generation of stds. to investigate the metabolism of DHA in tissues.

REFERENCE 4

AN 117:187518 CA
TI High-performance liquid chromatography-thermospray mass spectrometry of hydroperoxy polyunsaturated fatty acid acetyl derivatives
AU Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko; Ishikawa, Fumio
CS Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SO Journal of Chromatography (1992), 579(1), 25-36
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
AB A method for the anal. of hydroperoxy polyunsatd. fatty acids was developed. The hydroperoxy groups were acetylated by acetic anhydride, and the mixture was partially purified on a Sep-Pak C18 cartridge and

analyzed by high-performance liquid chromatog. with thermospray mass spectrometry. Generally, the base ion, [M + H - n(60)]+ or [M + H - n(60) - n(H2O)]+, is produced through elimination of acetic acid or water (n = number of hydroperoxy groups). The detection limit for these derivs. was approx. 1 pmol at concns. of hydroperoxy polyenoic acids prior to derivatization. Using this method, many hydroxy and hydroperoxy polyunsatd. fatty acid derivs. could be detected simultaneously within 30 min on a selected-ion monitoring detection chromatogram without a gradient system. The assay was successfully applied to hydroxy and hydroperoxy polyunsatd. fatty acids from an incubation mixture of rat brain homogenate to which polyunsatd. fatty acids has been added.

REFERENCE 5

AN 114:39806 CA
TI Stereochemical analysis of hydroxylated docosahexaenoates produced by human platelets and rat brain homogenate
AU Kim, H. Y.; Karanian, J. W.; Shingu, T.; Salem, N., Jr.
CS Sect. Anal. Chem., NIAAA, Bethesda, MD, 20892, USA
SO Prostaglandins (1990), 40(5), 473-90
CODEN: PRGLBA; ISSN: 0090-6980
DT Journal
LA English
AB The stereochem. configuration of hydroxylated products of docosahexaenoic acid (22:6ω3) formed by human platelets and rat brain homogenate were characterized for the first time. Chiral phase HPLC was employed along with autoxidized 22:6ω3 as reference material. The 14- and 11-hydroy 22:6ω3 (HDHE) products produced by human platelets were in the S configuration. Rat brain homogenate produced all of the 10 possible positional isomers when incubated with 22:6ω3. Their retention behavior on the reversed and chiral phase HPLC columns and GC/MS/EI anal. indicated that they were 20-, 17-, 16-, 14-, 13-, 11-, 10-, 8-, 7- and 4-HDHE. However, stereochem. anal. revealed that each positional isomer was a racemic mixture, suggesting that these were not formed by lipoxygenation but mainly by peroxidn. process.

REFERENCE 6

AN 101:35331 CA
TI Autooxidation of docosahexaenoic acid: analysis of ten isomers of hydroxydocosahexaenoate
AU VanRollins, Mike; Murphy, Robert C.
CS Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SO Journal of Lipid Research (1984), 25(5), 507-17
CODEN: JLPRAW; ISSN: 0022-2275
DT Journal
LA English
AB Docosahexaenoic acid, an n-3 essential fatty acid, is enzymically converted by platelets, basophils, and liver microsomes into metabolites containing conjugated diens with allylic hydroxyl groups. To help identify these metabolites, stds. were prepared by autoxidn. of docosahexaenoic acid. After isolation by reverse phase and normal phase high-performance chromatog. (HPLC), 10 hydroxy isomers of docosahexaenoic acid were identified by capillary gas-liquid chromatog., UV spectroscopy, and mass spectrometry. From these studies and reported elution orders for similar metabolites derived from linoleic, linolenic, and arachidonic acids, 2 basic HPLC elution patterns became apparent. Under reverse phase chromatog. conditions, the distance of the trans-double bond from the carboxyl group was the critical parameter in determining the elution order. Under silicic acid chromatog. conditions, the distance of the hydroxyl from the carbomethoxy group seemed to determine the elution order. The dramatic

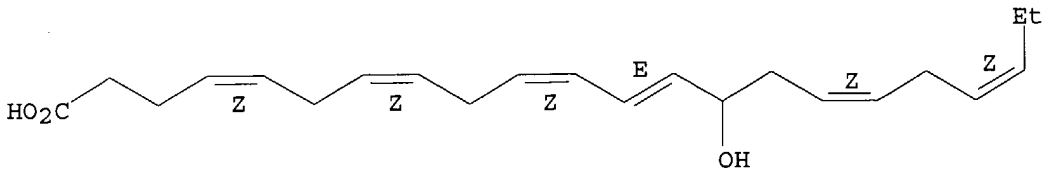
difference in selectivity between reverse and normal phase HPLC of the hydroxy acids provides critical information useful for identifying endogenous metabolites.

REFERENCE 7

AN 101:19194 CA
TI Oxidation of docosahexaenoic acid by rat liver microsomes
AU VanRollins, Mike; Baker, Rodney C.; Sprecher, Howard W.; Murphy, Robert C.
CS Health Sci. Cent., Univ. Colorado, Denver, CO, 80262, USA
SO Journal of Biological Chemistry (1984), 259(9), 5776-83
CODEN: JBCHA3; ISSN: 0021-9258
DT Journal
LA English
AB [1-14C]docosahexaenoic acid (n-3) was incubated at 37° for 30 min in the presence of rat liver microsomes and 1 mM NADPH. The products were isolated by using organic solvent extns., and reverse phase and normal phase HPLC. Isolates were identified by UV spectroscopy, capillary gas-liquid chromatog., and gas chromatog.-mass spectrometer. The major metabolites were: 19,20-, 16,17-, 13,14-, 10,11-, and 7,8-dihydroxydocosapentaenoic acids, 22-hydroxydocosahexaenoic acid, and 21-hydroxydocosahexaenoic acid. The minor metabolites were 17-hydroxy-4,7,10,13,15,19-, 16-hydroxy-4,7,10,17,19-, 14-hydroxy-4,7,10,12,-16,19-, 13-hydroxy-4,7,10,14,16,19-, 11-hydroxy-4,7,9,13,16,19-, 10-hydroxy-4,7,11,13,16,19-,8-hydroxy-4,6,10,13,16,19-, and 7-hydroxy-4,8,10,13,16,19-docosahexaenoic acids. These metabolites of docosahexaenoic acid resulted from 4 distinct classes of oxidation, ω-hydroxylations, (ω-1)-hydroxylations, epoxidns., and lipoxygenase-like hydroxylations. The similarity of these product profiles to those reported for comparable microsomal incubations with other essential fatty acids suggest that microsome cytochrome P 450 monooxygenases were involved.

L8 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2004 ACS on STN
RN **87042-40-8** REGISTRY
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (4Z,7Z,10Z,12E,16Z,19Z)-(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 4,7,10,12,16,19-Docosahexaenoic acid, 14-hydroxy-, (E,Z,Z,Z,Z,Z)-
FS STEREOSEARCH
DR 128302-08-9, 131485-68-2
MF C22 H32 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS, CSCHEM, TOXCENTER, USPAT2, USPATFULL
(*File contains numerically searchable property data)
DT.CA CAplus document type: Conference; Journal; Patent
RL.P Roles from patents: BIOL (Biological study); FORM (Formation, nonpreparative); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); OCCU (Occurrence); PREP (Preparation); PROC (Process)

Double bond geometry as shown.



10663061

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

32 REFERENCES IN FILE CA (1907 TO DATE)
32 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 139:79114 CA
TI Eicosapentaenoic acid and docosahexaenoic acid analogs induction of host defense against bacteria
IN Serhan, Charles N.; Colgan, Sean P.
PA The Brigham and Women's Hospital, USA
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003053423	A2	20030703	WO 2002-US40586	20021218
	WO 2003053423	A3	20040226		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US 2003191184	A1	20031009	US 2002-323867	20021218
	US 2003195248	A1	20031016	US 2002-323591	20021218

PRAI US 2001-342138P 20011218
AB Methods to cause tissue, such as mucosal cells, to express increased amts. of bactericidal permeability increasing protein (BPI) are described. Various BPI inducing agents include eicosapentaenoic acid (EPA) analogs and docosahexaenoic acid (DHA) analogs. Thus, 18R-EPA analogs induced the formation of BPI. Results demonstrated quant. PCR for BPI in epithelial cells.

REFERENCE 2

AN 136:147175 CA
TI Monohydroxylated fatty acid content in peripheral blood mononuclear cells and immune status of people at long times after the Chernobyl accident
AU Chumak, Anatoliy; Thevenon, Chantal; Gulaya, Nadya; Guichardant, Michel; Margitich, Victor; Bazyka, Dimitry; Kovalenko, Alexander; Lagarde, Michel; Prigent, Annie-France
CS INSERM, Biochimie et Pharmacologie INSA Lyon, Villeurbanne, 69621, Fr.
SO Radiation Research (2001), 156(5, Pt. 1), 476-487
CODEN: RAREAE; ISSN: 0033-7587
PB Radiation Research Society
DT Journal
LA English
AB The monohydroxylated fatty acid content of peripheral blood mononuclear cells from 23 cleanup workers and 16 unexposed individuals was studied in relation to their immune status after the Chernobyl accident. Men with absorbed doses below 0.32 Gy showed higher levels of free and esterified 12-hydroxyeicosatetraenoic acid (12-HETE) than unexposed men, whereas 15-HETE and the 17-hydroxy derivative of C22 fatty acid (17-OH 22), either

free or esterified in phospholipids, were increased in a dose-dependent manner. The percentage of CD4-pos. cells was also increased significantly in heavily irradiated men, whereas the percentage of CD8-pos. cells tended to decrease with dose. Furthermore, the absolute count of CD4-pos. cells was correlated pos. with the amount of esterified 15-HETE in the phospholipid fraction of the mononuclear cells and with the total 15-HETE. These results show for the first time that the accumulation of autoxidized/lipoxygenase products of polyunsatd. fatty acids in the mononuclear cells of irradiated individuals was associated with immune imbalance. This may be the basis for certain late effects of radiation such as autoimmune disorders, somatic and neoplastic diseases, and early aging.

RE.CNT 56 THERE ARE 56 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 3

AN 135:190408 CA
TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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	US 2002055538	A1	20020509	US 2001-785866	20010216
	US 6670396	B2	20031230		
	EP 1296923	A2	20030402	EP 2001-910912	20010216
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003525880	T2	20030902	JP 2001-559832	20010216
	US 2004059144	A1	20040325	US 2003-663061	20030912

PRAI US 2000-183078P 20000216
US 2000-238814P 20001006
US 2001-785866 20010216
WO 2001-US5196 20010216

AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of inflammation associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.

10663061

REFERENCE 4

AN 129:202364 CA
TI N-3 fatty acid deficiency in the rat pineal gland: effects on phospholipid molecular species composition and endogenous levels of melatonin and lipoxygenase products
AU Zhang, Hongjian; Hamilton, Jillonne H.; Salem, Norman, Jr.; Kim, Hee-Yong
CS Section of Mass Spectrometry, National Institute on Alcohol Abuse and Alcoholism, National Institutes of Health, Rockville, MD, 20852, USA
SO Journal of Lipid Research (1998), 39(7), 1397-1403
CODEN: JLPRAW; ISSN: 0022-2275
PB Lipid Research, Inc.
DT Journal
LA English
AB N-3 essential fatty acid deficiency affects a number of biol. and physiol. processes. In this study, the authors investigated the effect of n-3 essential fatty acid status on two key pineal biochem. functions, melatonin production and lipoxygenation, using pineal glands from rats given an n-3-adequate or n-3-deficient diet. The pineal total lipid profile and phospholipid mol. species distribution altered by n-3 deficiency were evaluated in parallel. In pineal glands from n-3-deficient rats, an 87% reduction of 22:6n-3 (docosahexaenoic acid) was observed, and this decrease was accompanied by increases in 22:4n-6 (docosatetraenoic acid, 3-fold), 22:5n-6 (docosapentaenoic acid, 12-fold), and 20:4n-6 (arachidonic acid, 48%). The significant decrease of 22:6n-3 containing species in phosphatidylcholine (PC), phosphatidylethanolamine (PE), and phosphatidylserine (PS) was also evident. These decreases in 22:6n-3 containing PL species were compensated by substantial accumulations of 22:4n-6 or 22:5n-6 and slight increases in 20:4n-6 containing PL species in PC and PE. In PS, however, the accumulation of n-6 species was not adequate to compensate for the loss of 22:6n-3 species. N-3 deficiency significantly reduced non-esterified 20:4n-6 and 22:6n-3 levels in pineals (25% and 65%, resp.). Concomitantly, the endogenous 12-HETE level decreased by 35% in deficient pineals. In contrast, n-3 deficiency led to a more than 60% increase in the daytime pineal melatonin level. In conclusion, n-3 fatty acid deficiency not only has profound effects on pineal lipid profiles but also on pineal biochem. activities. These results suggest that n-3 fatty acids may play a critical role in regulating pineal function.
RE.CNT 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

REFERENCE 5

AN 124:227170 CA
TI Production of monohydroxy derivatives from highly unsaturated fatty acids in the gills of red sea bream Pagrus major
AU Iijima, Noriaki; Hada, Takahiko; Kayama, Mitsu
CS Faculty of Applied Biological Science, Hiroshima Univ., Hiroshima, 739, Japan
SO Fisheries Science (1996), 62(1), 114-21
CODEN: FSCIEH; ISSN: 0919-9268
PB Japanese Society of Fisheries Science
DT Journal
LA English
AB 12-Hydroxyeicosatetraenoic acid and 15-hydroxyeicosatetraenoic acid were produced as major and minor monohydroxylated products in a microsome fraction, when [1-14C]arachidonic acid was incubated with the microsome or cytosol fraction prepared from frozen stored gill tissue of red sea bream P. major. The endogeneous products extracted from the microsome fraction of the red sea bream gill were isolated by HPLC and identified as 12-hydroxyeicosatetraenoic acid, 12-hydroxyeicosapentaenoic acid, and

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14-hydroxydocosahexaenoic acid by UV absorption spectrometry and gas chromatog.-mass spectrometry. These data suggest that arachidonic acid, eicosapentaenoic acid, and docosahexaenoic acid are converted to their monohydroxy derivs. via the hydroperoxides by the action of 12-lipoxygenase-like enzyme, which is distributed in the microsomes of red sea bream gill.

REFERENCE 6

AN 124:26230 CA
TI Biosynthesis of docosanoids by human platelet: Cardiovascular properties
AU Karanian, John W.; Kim, Hee Yong; Salem, Norman Jr.
CS Laboratory Membrane Biochemistry and Biophysics, DICBR/NIAAA, Rockville, MD, 20852, USA
SO Cardiovascular Disease 2: Cellular and Molecular Mechanisms, Prevention, and Treatment, [Proceedings of the Washington International Spring Symposium], 14th, Washington, D. C., June 6-10, 1994 (1995), Meeting Date 1994, 269-77. Editor(s): Gallo, Linda L. Publisher: Plenum, New York, N. Y.
CODEN: 61ZNA9
DT Conference
LA English
AB A reliable purification and quantification method is presented that was used to characterize the metabolism and production of the hydroxylated derivs. of 22:5n3, 22:6n3, 22:5n5 and 22:5n6 from mammalian platelets. Their biol. properties in platelet and vascular smooth muscle cell function is discussed.

REFERENCE 7

AN 122:311127 CA
TI Eicosanoid generating capacities of different tissues from the rainbow trout, Oncorhynchus mykiss
AU Knight, John; Holland, Jason W.; Bowden, Linda A.; Halliday, Katrina; Rowley, Andrew F.
CS School Biological Sciences, University Wales, Swansea, Singleton Park, SA2 8PP, UK
SO Lipids (1995), 30(5), 451-8
CODEN: LPDSAP; ISSN: 0024-4201
PB AOCS Press
DT Journal
LA English
AB The eicosanoid-generating potential of the brain, gills, skin, ovary, muscle, eye, liver, spleen, heart, and alimentary canal in the rainbow trout, O. mykiss, was examined All the organs/tissues examined synthesized the 12-lipoxygenase products, 12-hydroxyeicosatetraenoic acid (12-HETE), and 12-hydroxyeicosapentaenoic acid (12-HEPE), implying the widespread nature of this enzyme in trout. Both prostaglandin E and LTC were also found in variable amts. in the organs, with the greatest amount of PGE found in the gill. Leukotriene (LT) B4 and LTB5 were found in supernatants from Ca2+ ionophore-challenged brain, skin, ovary, liver, spleen, and heart, but the lipoxins A4 and A5 were only present in brain, ovary, and spleen in relatively small amts. As lipoxins have previously been shown to be synthesized by macrophages in rainbow trout, and related cells (microglial cells) are found in the brain of mammals, the localization of macrophage-like cells in trout brain was investigated immunocytochem. Monoclonal antibodies specific for trout leukocytes failed to identify any microglial-like cells in sections of the brain, although microvessels containing immuno-pos. reaction products were observed A number of distinct lipoxygenase products were found in supernatants of ionophore-challenged gill, including 14-hydroxydocosahexaenoic acid, 12-HETE, and 12-HEPE, and

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a large number of dihydroxy fatty acid derivs. with conjugated triene chromophores. One of these products was tentatively identified as 8(R),15(S)-dihydroxyeicosatetraenoic acid, a dual 12- and 15-lipoxygenase product, but apparently no LTB4 was generated by this tissue.

REFERENCE 8

AN 121:277471 CA
TI Inhibitory effects of n-6 and n-3 hydroxy fatty acids on thromboxane (U46619)-induced smooth muscle contraction
AU Karanian, J. W.; Kim, H. Y.; Salem, Norman, Jr.
CS Lab. Membrane Biochem. and Biophysics, Natl. Inst. Alcohol Abuse and Alcoholism, Bethesda, MD, USA
SO Journal of Pharmacology and Experimental Therapeutics (1994), 270(3), 1105-9
CODEN: JPETAB; ISSN: 0022-3565
DT Journal
LA English
AB Mammalian platelets are capable of enzymically producing a number of n-6 and n-3 hydroxy fatty acids. Human platelet suspensions produce two major docosahexaenoic acid (22:6n3) metabolites, namely, 11-OH- and 14-OH-22:6n3. The hydroxy fatty acids which were formed by human platelets and purified by high performance liquid chromatog. specifically antagonize the contractile effects of a thromboxane mimetic, U46619, in airway, visceral and, especially, in the vascular smooth muscle prepns. studied.
The efficacy of OH-22:6n3 (IC25 = 1.1 μM) was compared to other n-6 and n-3 hydroxy fatty acids in the rat aortic ring preparation The OH-22:6n3 was significantly more potent with the exception of OH-22:5n3. The rank order of their potency was 14-OH-22:5n3 ≥ 14-OH-22:6n3 > 17-OH-22:6n3 ≥ 11-OH-22:6n3 ≥ 11-OH-22:5n3 > 12-OH-20:5n3 ≥ 12-OH-20:4n6 ≥ 14-OH-22:5n6 > 13-OH-18:2n6 > 14-OH-22:5n5. Antagonism of thromboxane effects may be an important aspect of the biol. function of 22-carbon n-3 hydroxylated fatty acids in the platelet-vascular smooth muscle cell interactions.

REFERENCE 9

AN 121:73909 CA
TI Antipsychotics containing docosahexaenoic acid or its derivatives
IN Nishikawa, Masazumi; Kimura, Seiji
PA Maruha Kk, Japan
SO Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 06072868	A2	19940315	JP 1992-227510	19920826
	US 6306907	B1	20011023	US 1993-111831	19930825

PRAI JP 1992-227510 19920826
AB Antipsychotics contain ≥1 compds. chosen from docosahexaenoic acid (I) or its derivs. as active ingredients, which show high safety and are useful for prevention and treatment of psychosis. I at 30 μM reduced N-methyl-D-aspartic acid receptor antagonism of phencyclidine in hippocampus CA1 region nerve cell sample of sliced rat brain. Et docosahexaenoate at 300 mg 3 times a day improved neg. symptoms in schizophrenia patients and showed no side effects.

REFERENCE 10

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AN 120:265249 CA
TI High-performance liquid chromatography-thermospray mass spectrometry of epoxy polyunsaturated fatty acids and epoxyhydroxy polyunsaturated fatty acids from an incubation mixture of rat tissue homogenate
AU Yamane, Mototeru; Abe, Akihisa; Yamane, Sayoko
CS Dep. Biochem., Tokyo Med. Coll., Tokyo, Japan
SO Journal of Chromatography, B: Biomedical Sciences and Applications (1994), 652(2), 123-36
CODEN: JCBBEP; ISSN: 1387-2273
DT Journal
LA English
AB A method for the anal. of epoxy polyunsatd. fatty acids (EpPUFAs) and epoxyhydroxy polyunsatd. fatty acids (EpHPUFAs) in rat tissue homogenate, with homo-γ-linolenic acid (20:3,n-6), arachidonic acid (20:4,n-6), eicosapentaenoic acid (20:5,n-3) or docosahexaenoic acid (22:6,n-3) as a substrate, was developed. Extraction with dichloromethane at pH 4-5 and concentration in the presence of pyridine were performed. Spectral anal. of chromatograms obtained with HPLC-thermospray mass spectrometry showed the presence of EpPUFAs, EpHPUFAs and dihydroxy metabolites (DiHPUFAs) of EpPUFAs corresponding to each precursor fatty acid. On a selected-ion monitoring chromatogram, many EpPUFAs, EpHPUFAs and DiHPUFAs in an extract from an incubation mixture of each precursor fatty acid in aged rat tissue homogenate were detected simultaneously within 70 min. EpPUFAs and DiHPUFAs derived from 20:3 (n-6) or 20:5 (n-3) were detected in significant amts. From these results, a highly active cytochrome P 450 system or nonenzymic oxidative reactions in aged rat tissue homogenate were suggested.

=> file ca

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	30.60	30.81

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-3.96	-3.96

FILE 'CA' ENTERED AT 11:54:16 ON 27 SEP 2004

FILE COVERS 1907 - 23 Sep 2004 VOL 141 ISS 14
FILE LAST UPDATED: 23 Sep 2004 (20040923/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

10663061

Ref. Inflammation
Related to part. Compd

=> s l8
L9 36 L8

=> s l9 and inflammation
106668 INFLAMMATION
L10 2 L9 AND INFLAMMATION

=> d 1-2 l10 bib abs

L10 ANSWER 1 OF 2 CA COPYRIGHT 2004 ACS on STN
AN 139:177077 CA
TI Novel Docosatrienes and 17S-Resolvins Generated from Docosahexaenoic Acid in Murine Brain, Human Blood, and Glial Cells
AU Hong, Song; Gronert, Karsten; Devchand, Pallavi R.; Moussignac, Rose-Laure; Serhan, Charles N.
CS Perioperative and Pain Medicine, Department of Anesthesiology, Center for Experimental Therapeutics and Reperfusion Injury, Brigham and Women's Hospital and Harvard Medical School, Boston, MA, 02115, USA
SO Journal of Biological Chemistry (2003), 278(17), 14677-14687
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
AB Docosahexaenoic acid (DHA, C22:6) is highly enriched in brain, synapses, and retina and is a major ω-3 fatty acid. Deficiencies in this essential fatty acid are reportedly associated with neuronal function, cancer, and **inflammation**. Here, using new lipid analyses employing high performance liquid chromatog. coupled with a photodiode-array detector and a tandem mass spectrometer, a novel series of endogenous mediators was identified in blood, leukocytes, brain, and glial cells as 17S-hydroxy-containing docosanoids denoted as docosatrienes (the main bioactive member of the series was 10,17S-docosatriene) and 17S series resolvins. These novel mediators were biosynthesized via epoxide-containing intermediates and proved potent (pico- to nanomolar range) regulators of both leukocytes reducing infiltration in vivo and glial cells blocking their cytokine production These results indicate that DHA is the precursor to potent protective mediators generated via enzymic oxygenations to novel docosatrienes and 17S series resolvins that each regulate events of interest in **inflammation** and resolution
RE.CNT 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 2 OF 2 CA COPYRIGHT 2004 ACS on STN
AN 135:190408 CA
TI Aspirin-triggered lipid mediators
IN Serhan, Charles N.; Clish, Clary B.
PA The Brigham and Women's Hospital, Inc., USA
SO PCT Int. Appl., 74 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001060778	A2	20010823	WO 2001-US5196	20010216
	WO 2001060778	C2	20021024		
	WO 2001060778	A3	20030116		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU,

ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

US	2002055538	A1	20020509	US 2001-785866	20010216
US	6670396	B2	20031230		
EP	1296923	A2	20030402	EP 2001-910912	20010216
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP	2003525880	T2	20030902	JP 2001-559832	20010216
US	2004059144	A1	20040325	US 2003-663061	20030912
PRAI US	2000-183078P	P	20000216		
US	2000-238814P	P	20001006		
US	2001-785866	A3	20010216		
WO	2001-US5196	W	20010216		

OS MARPAT 135:190408

AB Aspirin triggered lipid mediators are disclosed which are useful for the treatment or prevention of **inflammation** associated with various diseases, including ischemia. The present invention provides that inflammatory exudates from mice treated with ω-3 PUFA and aspirin generate a novel array of bioactive lipid signals. Human endothelial cells with upregulated COX-2 treated with aspirin converted C20:5 w-3 to 18R-HEPE and 15R-HEPE. Each was used by polymorphonuclear leukocytes to generate sep. classes of novel trihydroxy-containing mediators, including 15R-lipoxin and 5,12,18R-triHEPE. These compds. were potent inhibitors of human polymorphonuclear leukocyte transendothelial migration and infiltration in vivo.